

Global-Micro Approaches for Elasto-Plastic Short Transient Applications on Scalable Computers

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- Theoretical Developments
- Preliminary Serial Code

Objective

- Strategies for making a macro-micro analysis parallel
 - within the context of asymptotic homogenization method
 - macro/global analysis based on explicit formulation
 - micro/local analysis based on implicit formulation

Outline

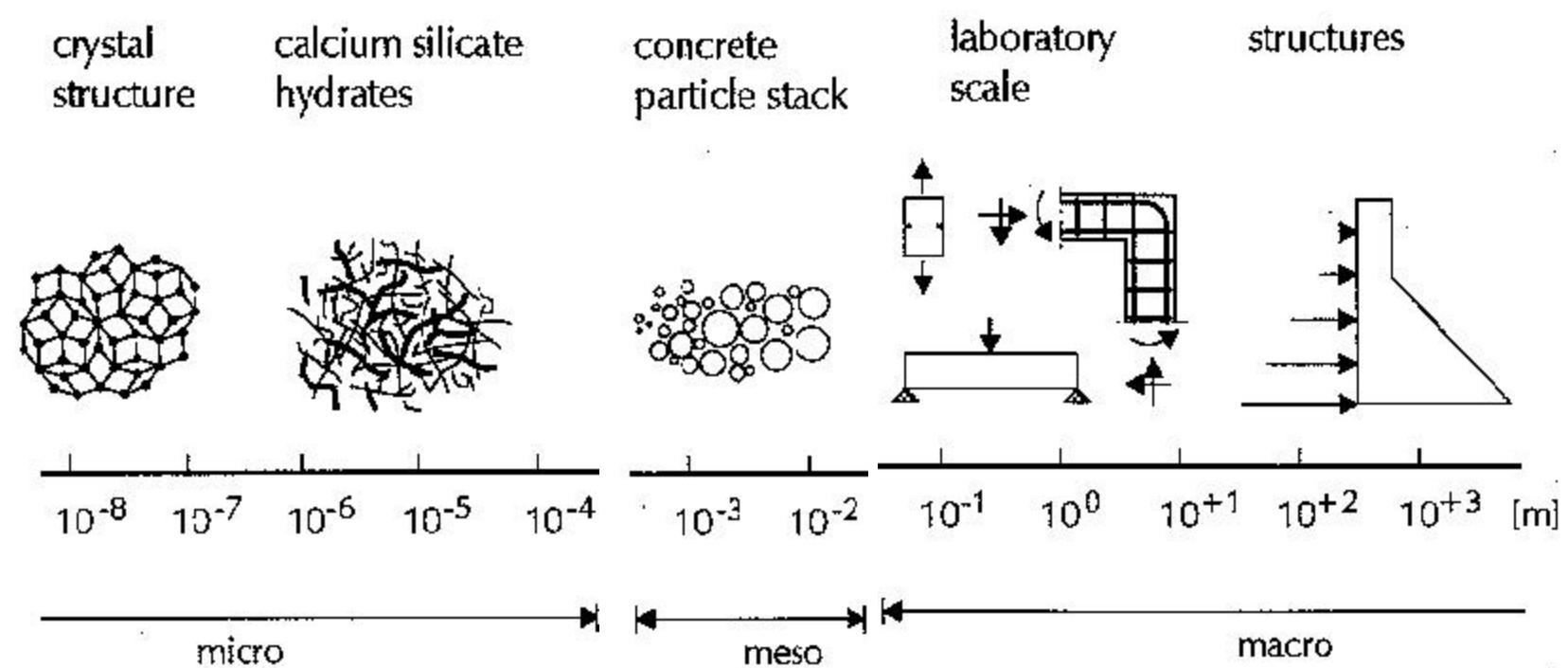
Multiscale-analysis

AEH

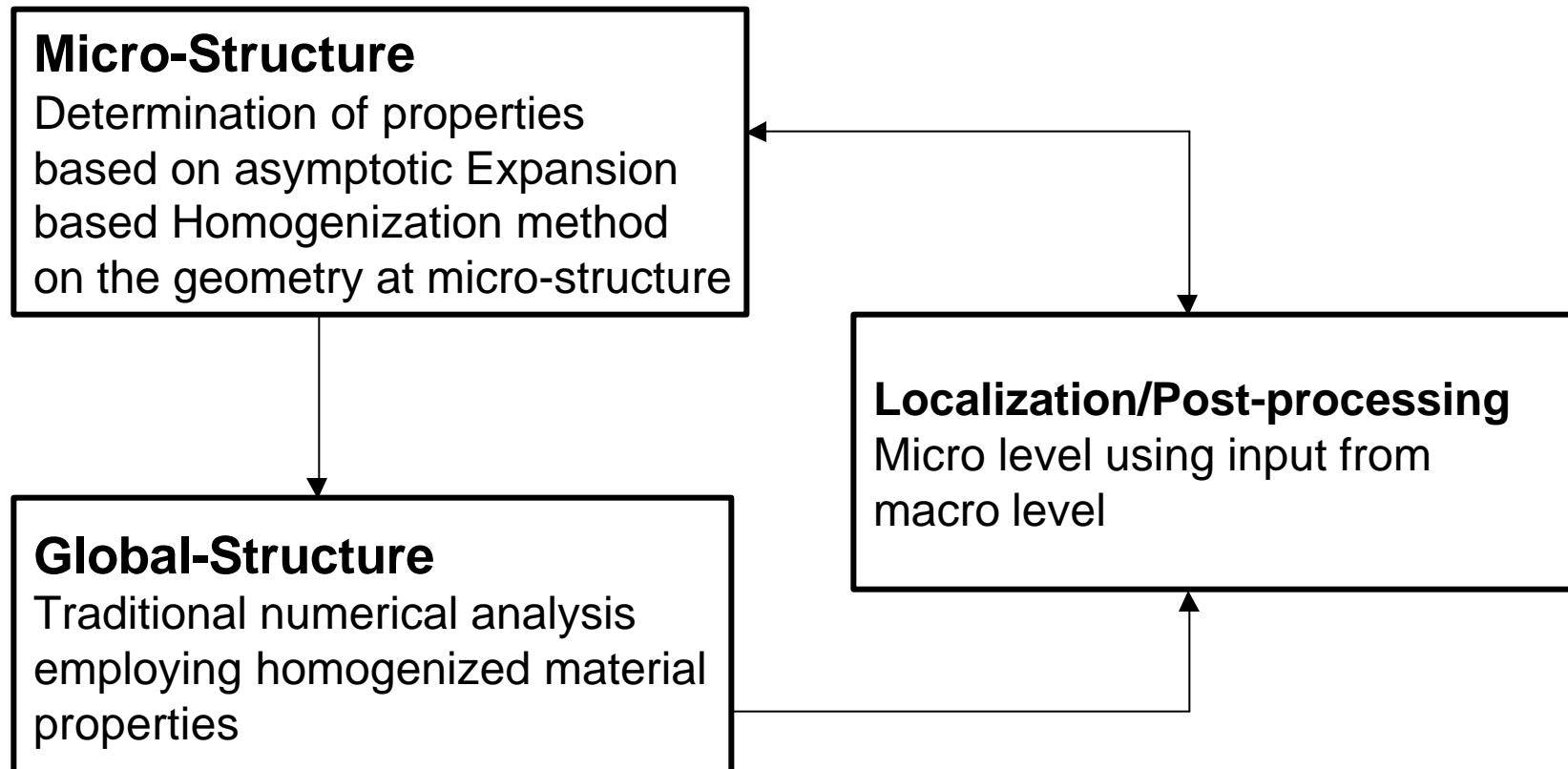
Parallelization Strategies

Results and Conclusions

Different length scales for Concrete



Asymptotic Expansion Homogenization (AEH)



Asymptotic Expansion Homogenization Procedure

- **Solve microscopic equilibrium equation with periodic boundary conditions, then obtain the characteristic deformations**
- **Evaluate homogenized material properties**
- **Solve the global equilibrium equations, then obtain global displacements**
- **Evaluate microscopic stresses using global strains**

Micromechanical equations: Asymptotic Expansion Homogenization

$$v_i^\varepsilon(\mathbf{x}, \mathbf{y}) = v_{0_i}(\mathbf{x}, \mathbf{y}) + \varepsilon v_{1_i}(\mathbf{x}, \mathbf{y}) + \varepsilon^2 v_{2_i}(\mathbf{x}, \mathbf{y}) + \dots$$

$$\begin{aligned}\dot{e}_{ij}^\varepsilon(\mathbf{x}, \mathbf{y}) &= [e_{ij}^x(v_0) + e_{ij}^y(v_1)] \\ &\quad + \varepsilon [e_{ij}^x(v_1) + e_{ij}^y(v_2)] + \dots\end{aligned}$$

Applying averaging principal with the limit $\varepsilon \rightarrow 0$, the microscopic velocities are

$$v_{1_i}^{n-1} = -\chi_i^{mn} \frac{\partial v_{0_m}^{n-1}}{\partial x_n} - \frac{1}{\Delta t} \chi_i^2 + \tilde{v}_{1_i}(x)$$

Microscopic equilibrium equations

$$\begin{aligned}\frac{\partial}{\partial y_j} C_{ijkl}^* \frac{\partial \chi_k^{mn}}{\partial y_l} &= \frac{\partial}{\partial y_j} C_{ijmn}^* \\ \frac{\partial}{\partial y_j} C_{ijkl}^* \frac{\partial \chi_k^2}{\partial y_l} &= \frac{\partial}{\partial y_j} \left(M_{ijkl} \sigma_{kl}^{\varepsilon^{n-\frac{1}{2}}} \right)\end{aligned}$$

Global Equations

$$\rho^\varepsilon \dot{v}_i^\varepsilon - \sigma_{ji,j}^\varepsilon = f_i$$

$$\rho v_i^{\varepsilon^{n+1}}-\rho v_i^{\varepsilon^n}=\sigma_{ji,j}^{\varepsilon^{n+\frac{1}{2}}}+\rho f_i^{n+\frac{1}{2}}$$

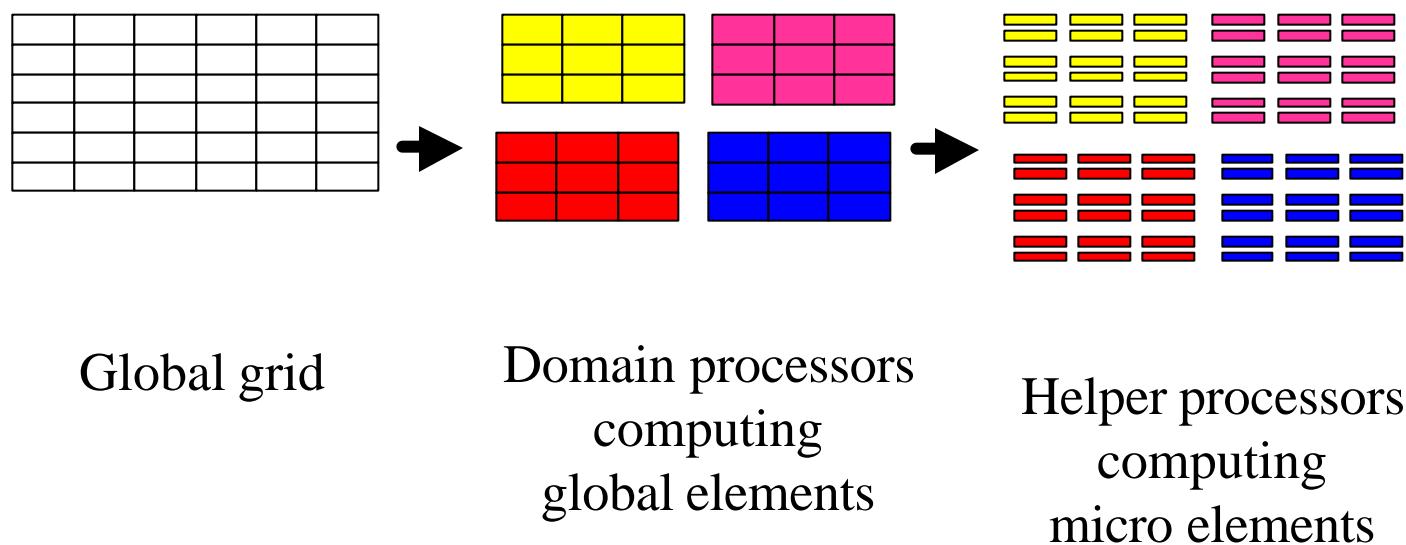
$$\sigma_{ij}^{\varepsilon^{n+\frac{1}{2}}}=M_{ijkl}\left(\sigma_{kl}^{\varepsilon^{n-\frac{1}{2}}}+C_{klmn}\dot{\epsilon}^{\varepsilon^{n-\frac{1}{2}}}\Delta t\right)$$

$$\left\langle\rho\right\rangle\Delta v_{0_i}^{n+1}=\Delta t\frac{\partial}{\partial x_j}\left\langle\sigma_{ij}^{n+\frac{1}{2}}-\sigma_{ij}^c\right\rangle+\Delta t\left\langle\rho\right\rangle f_i^{n+\frac{1}{2}}$$

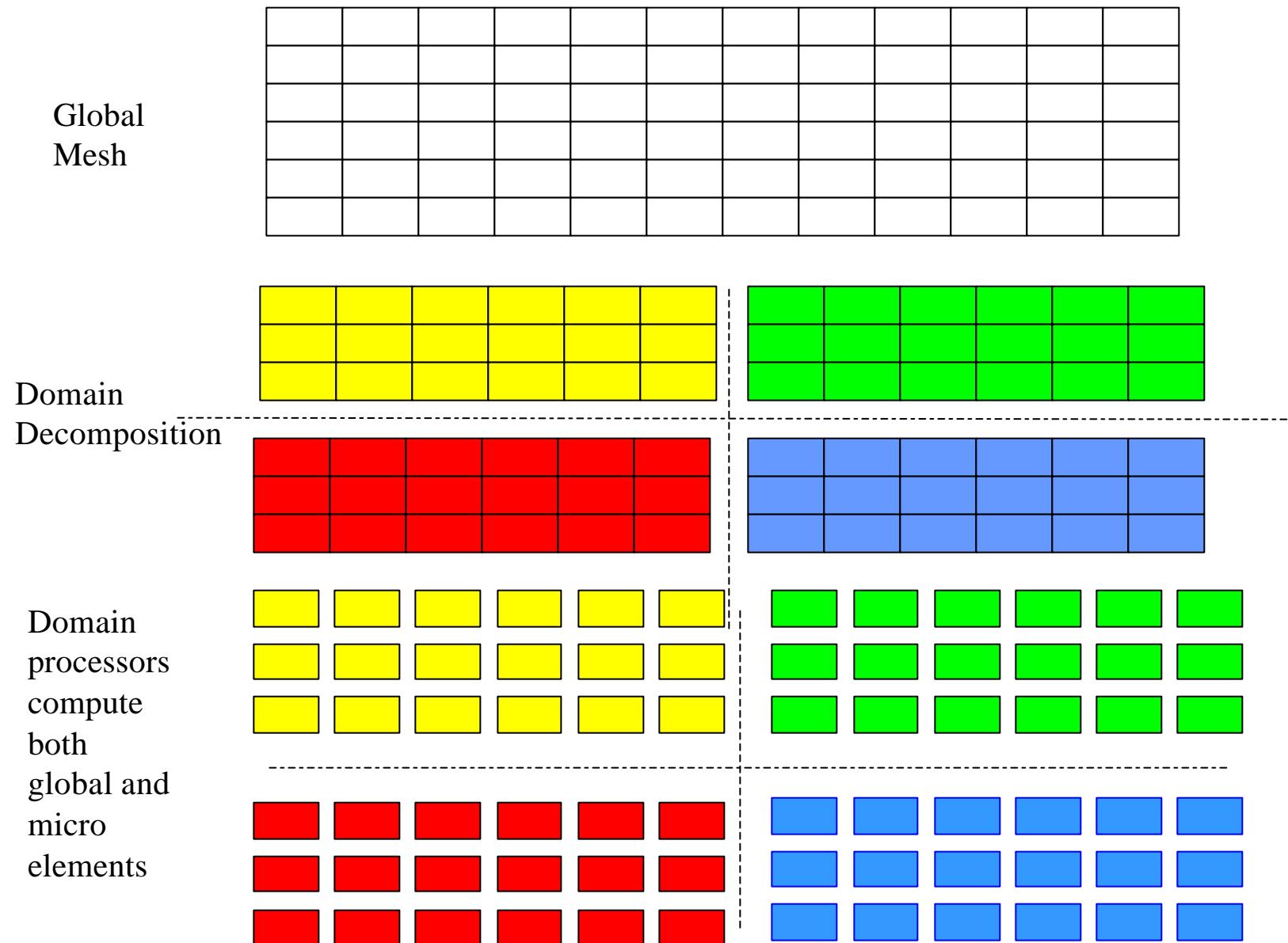
$$\sigma_{ij}^c=C_{ijkl}^*\left(\frac{\partial\chi_k^2}{\partial y_l}+\frac{\partial\chi_k^{mn^1}}{\partial y_l}\frac{\partial v_{0_m}^{n-1}}{\partial x_n}\Delta t\right)$$

$$\langle (\quad)\rangle = \frac{1}{V}\int_Y (\quad) dY$$

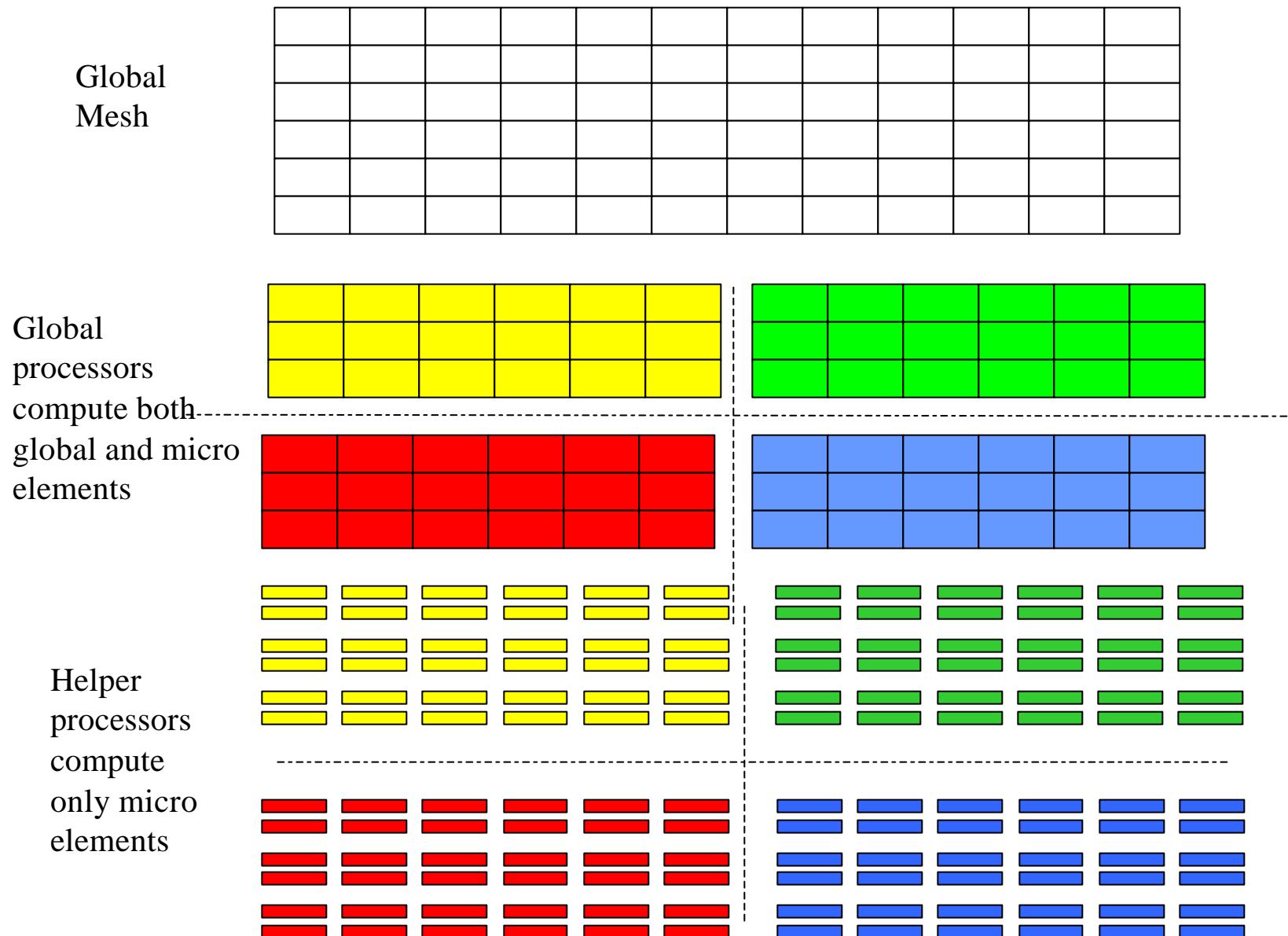
SCALABLE IMPLEMENTATION OF AEH



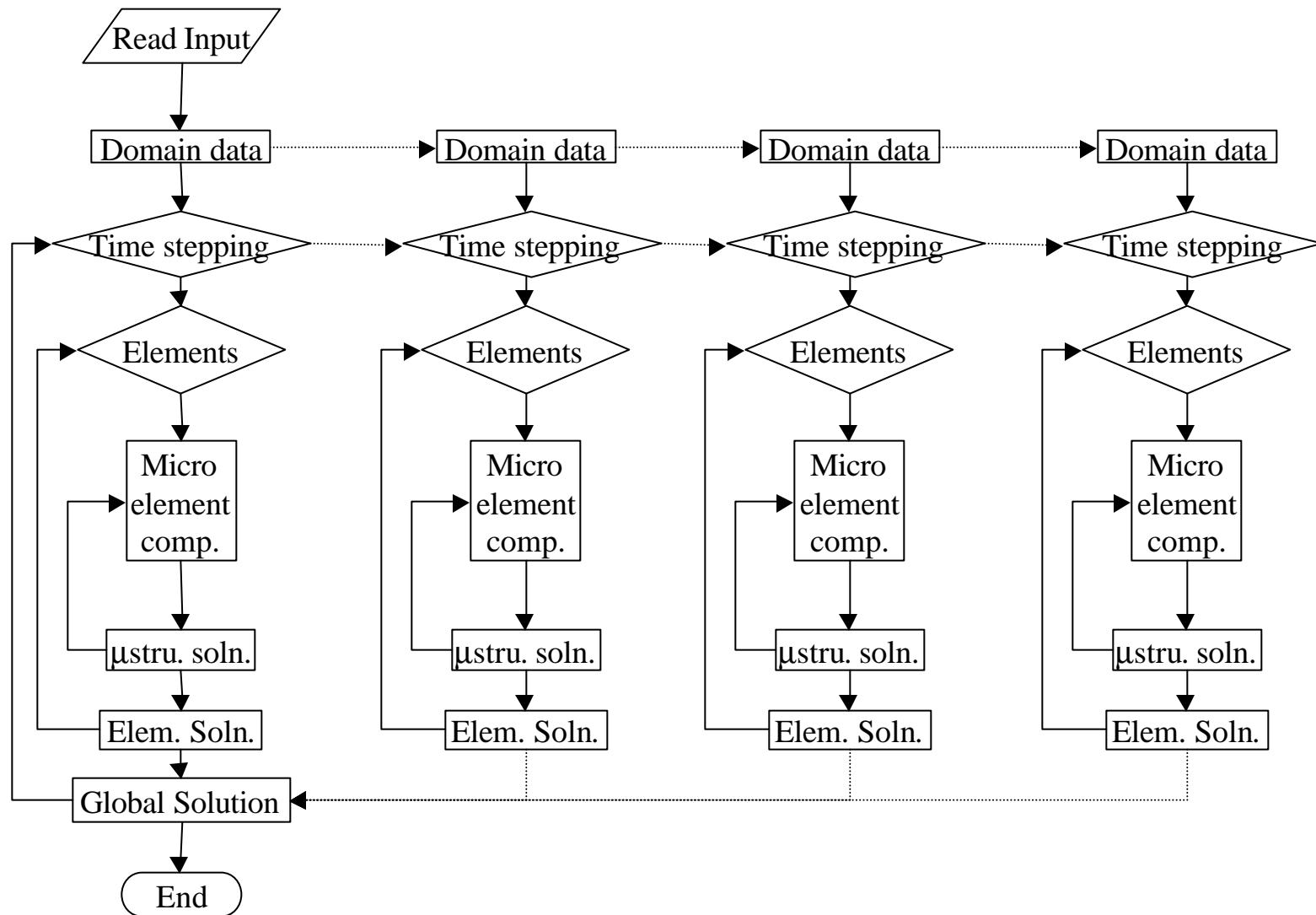
Strategy 1



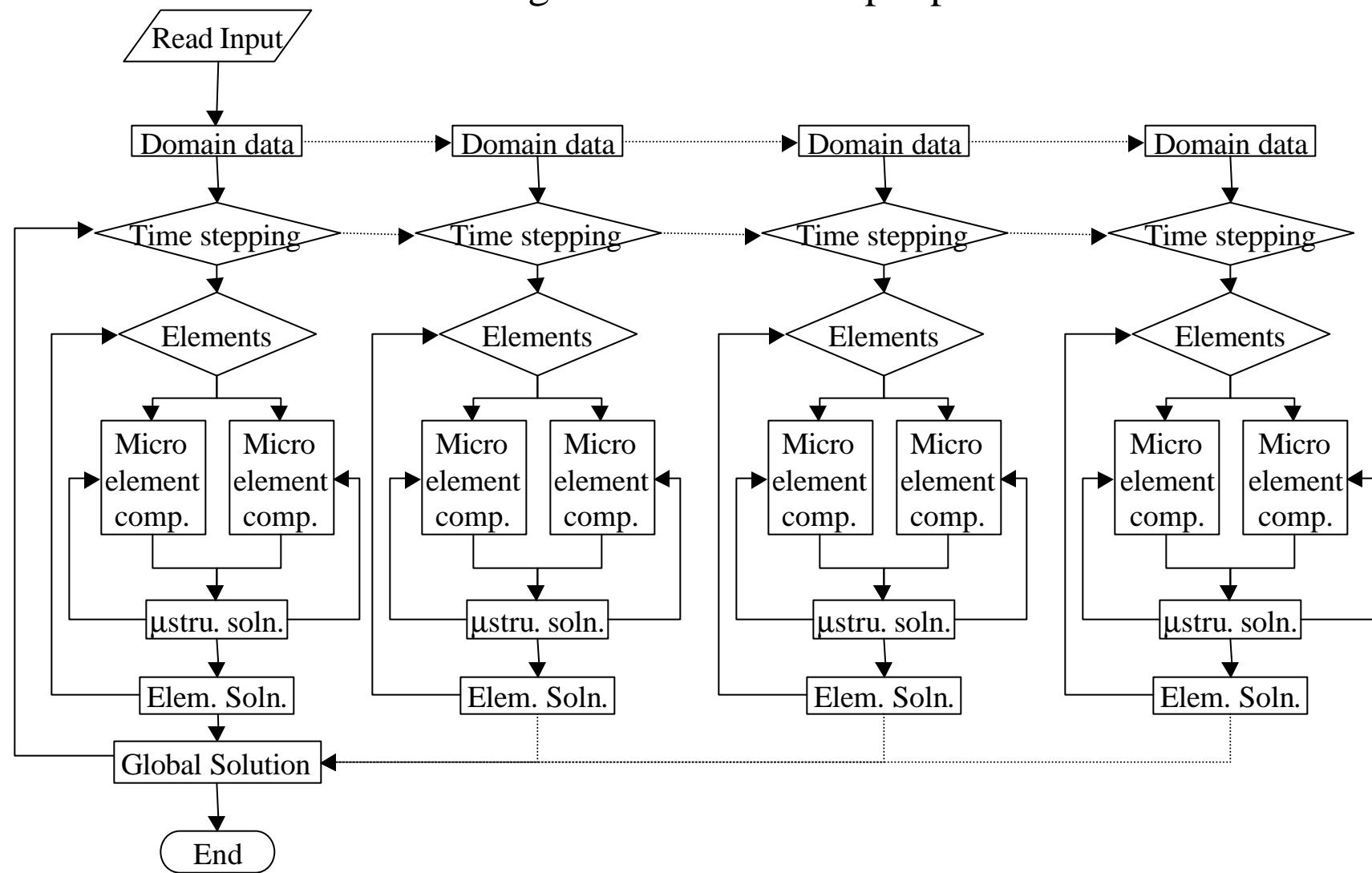
Strategy 2



Program Flow w/o helper processors

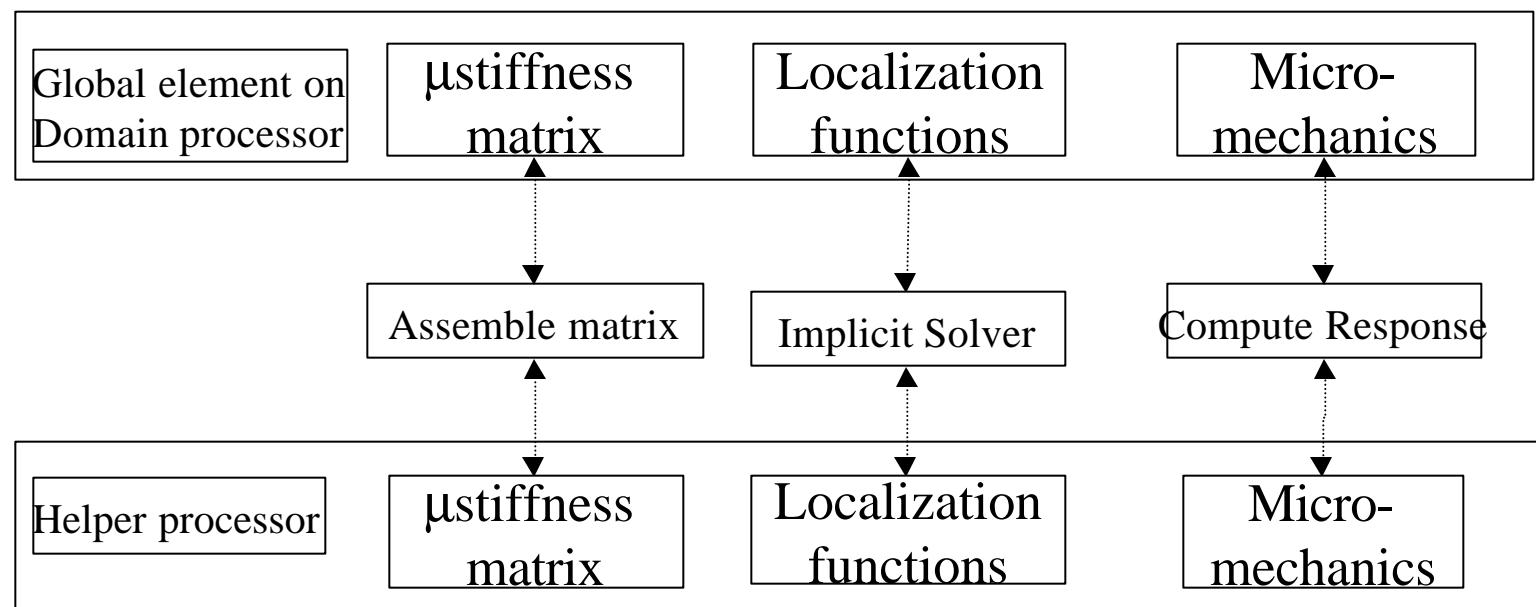


Program Flow with helper processors



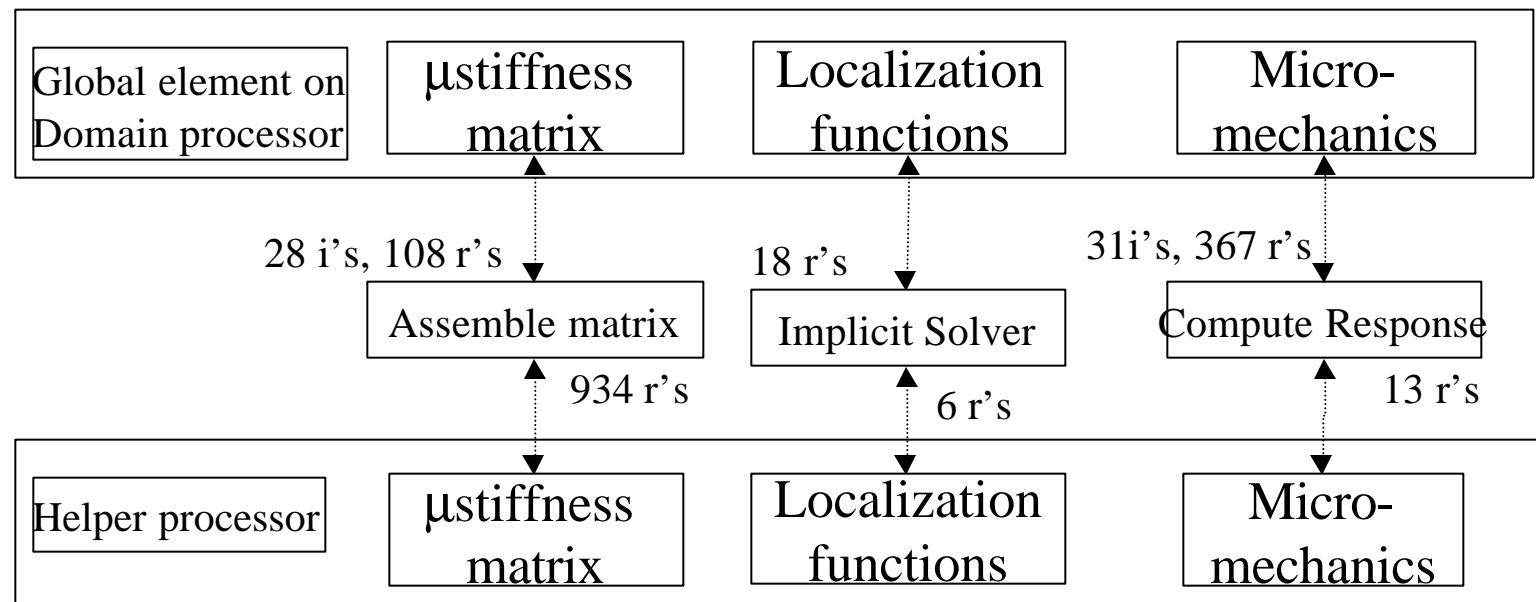
3 μelement computation areas

1. Computation and assembly of micro-stiffness matrices
2. Implicit solution of the Localized functions
3. Aggregation of the macro element response from the μelement stresses.



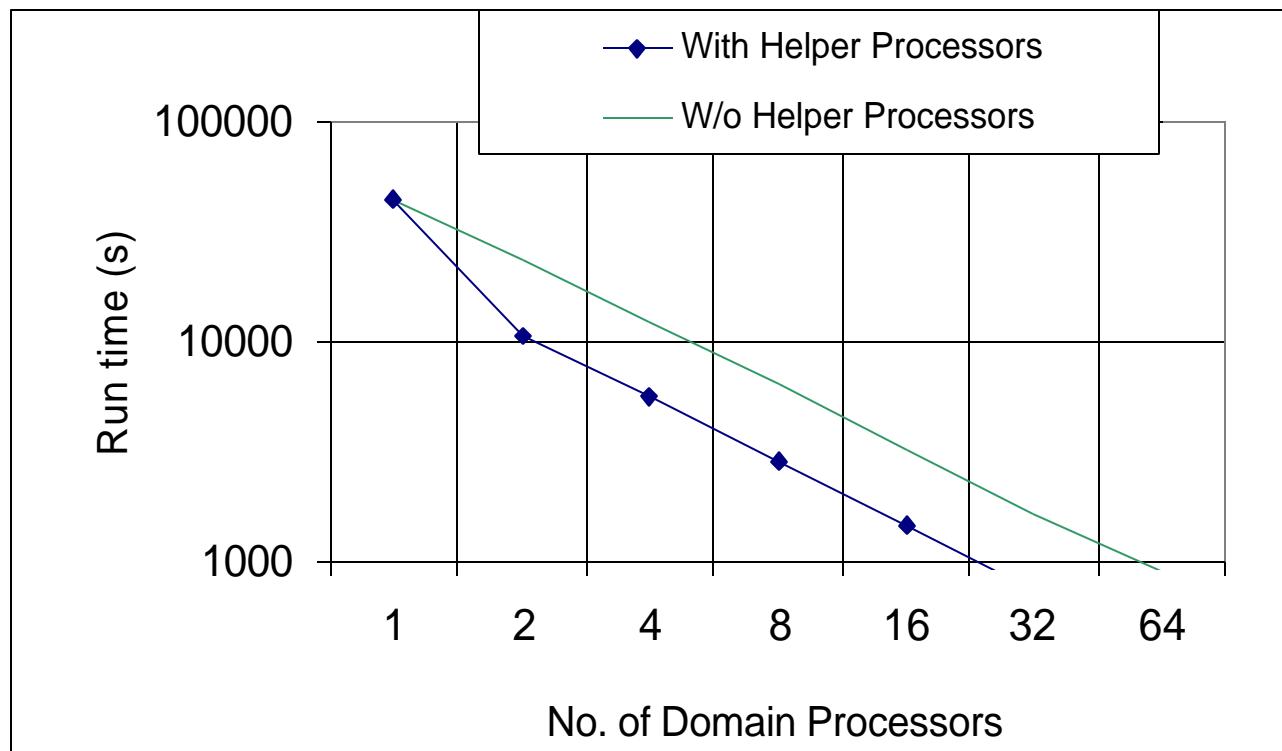
Communication buffer sizes for the μ element computation areas

1. Computation and assembly of micro-stiffness matrices
2. Implicit solution of the Localized functions
3. Aggregation of the macro element response from the μ element stresses.



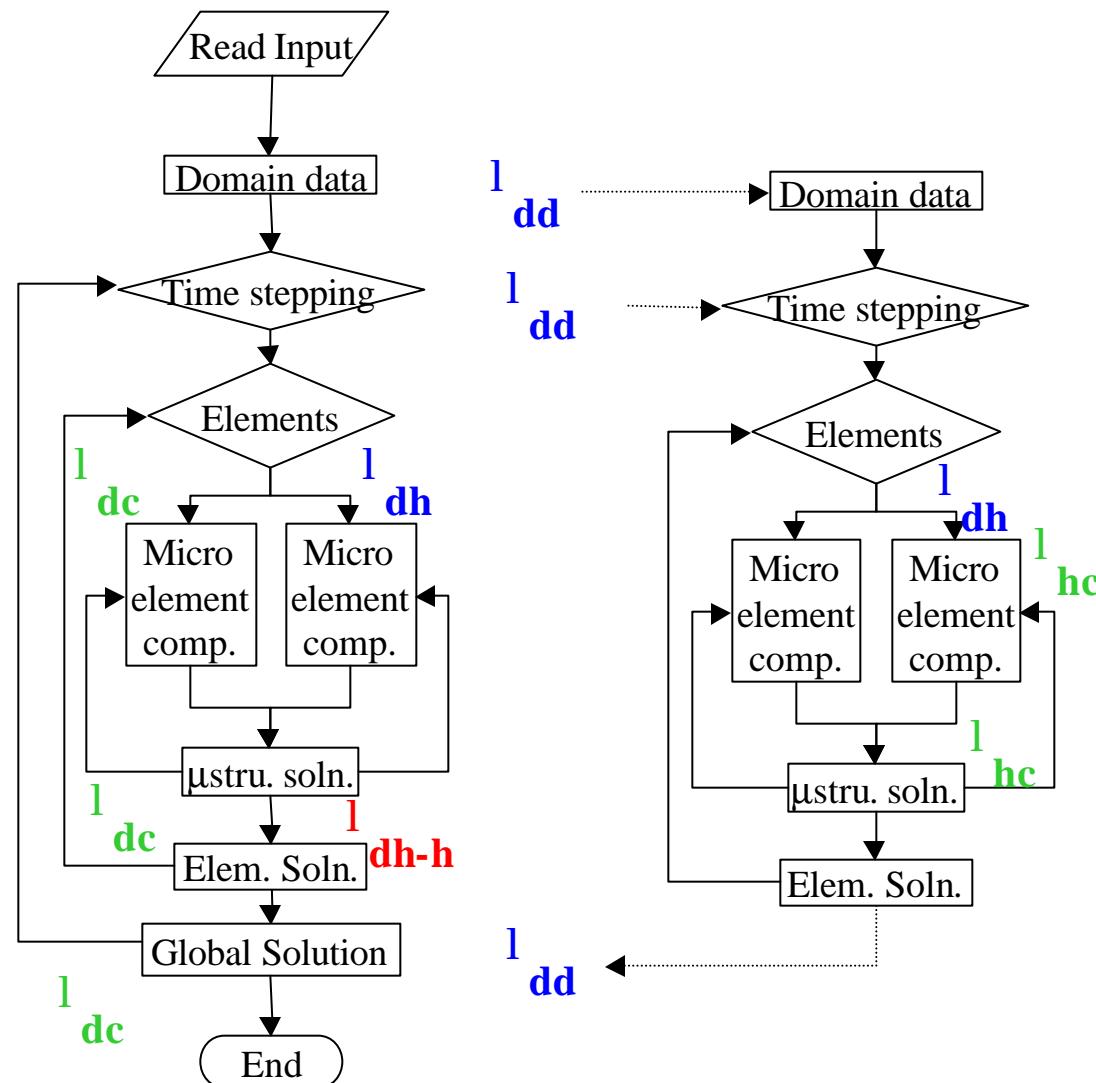
HPC Computer Resources

- MPI paradigm
- SCALAPACK
PDGESV implicit solver for μelement solution
- herman@arl.hpc.mil
(a 128 processor 300 MHZ SGI origin 2000)
- adele@arl.hpc.mil
(a 64 processor 300 MHZ SGI origin 2000)



Total run times vs. total number of domain processors for the two strategies

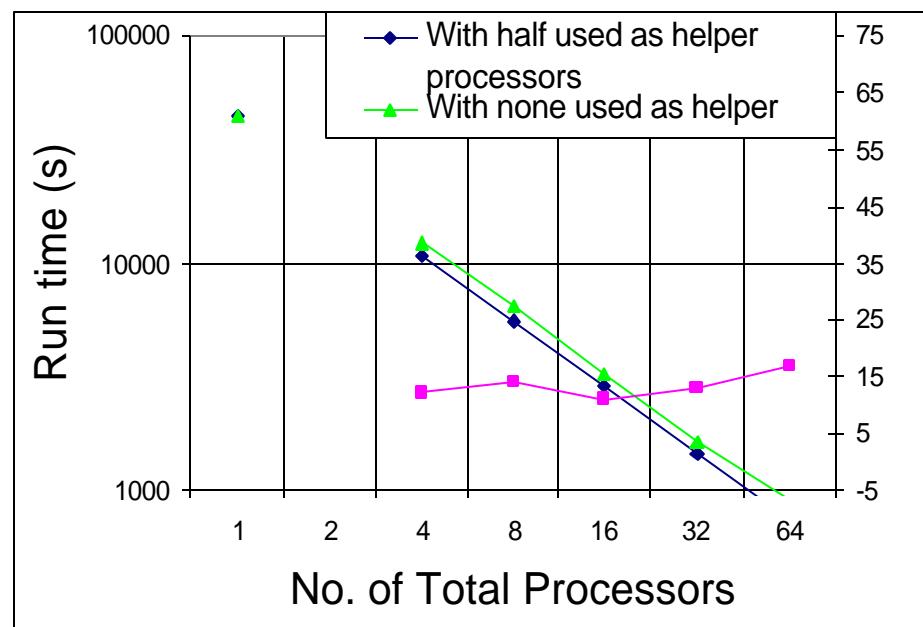
Computation, communication and wait times



Total vs. effective run times

	Comp.	Wait	Comm.	Comm.
Domain Proc.	λ_{dc}	λ_{dw}	λ_{dd}	
Helper Proc.	λ_{hc}	λ_{hw}	λ_{dh-d}	λ_{dh-h}

Strategy	Total run time	Effective run time	η
1	$\lambda_1 = \lambda_{dc} + \lambda_{dd} + \lambda_{dw}$	$\lambda_{11} = \lambda_{dc} + \lambda_{dd}$	
2	$\lambda_2 = \lambda_{dc} + \lambda_{dd} + \lambda_{dw}$ $+ \lambda_{hc} + \lambda_{hw}$ $dh-d dh-h$	$\lambda_{21} = \lambda_{dc} + \lambda_{dd}$ $+ \lambda_{hc} + \lambda_{dh-h}$ $dh-d dh-h$	$(\lambda_{21}/\lambda_{11} - 1) * 100$



Total run times vs. total number of processors for the two strategies

How best to deploy the idle processors
to help the ongoing **computations** at other processors



**Computation intensive
in a few processors**

**Communication intensive
across processors**

Decompositions sometimes neglects equitable distribution of elements
undergoing plasticity and large deformation

CONCLUDING REMARKS

- Microelement computations are a significant part of total run time.
- Total run time reduces when some processors are used in helper mode
- Helper processors' communication time is significant;
but it scaled fairly with the number of processors.
- Helper processors' wait time is considered not a problem;
OpenMP and MPI2 allow dynamic spawning of processes.
- Future Effort:
Very large microstructures
microstructure response using explicit formulation-theoretical development